Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Students' Annual Seminar

Prediction of Photo-electron Spectroscopy by excitation of core-electrons

Susmita Tripathy

X-ray spectroscopic techniques are widely used for characterising materials and surfaces. While the experimental spectra obtained can provide information for a given molecule, theoretical simulations of excitations corresponding to photoemission are necessary to disambiguate individual spectral assignments and for understanding the contribution of individual atoms to the peaks. In this talk, we will discuss the modelling of XPS and NEXAFS by constraining core-holes in molecular systems and emphasise on how to deal with relaxation effects due to the core-hole. Additionally, we will explore the role of the local atomic environment in shaping individual peaks and demonstrate how machine learning can be utilised to accurately describe 1s core binding energies for the QM9 dataset.

Friday, Mar 31st 2023

10:00 AM (Tea / Coffee 9.45 AM)

Seminar Hall, TIFR-H